### Improved Simulation of Lightning-Produced Nitrogen Oxides, Convective Transport, and Their Effects on Upper Tropospheric Ozone Concentrations

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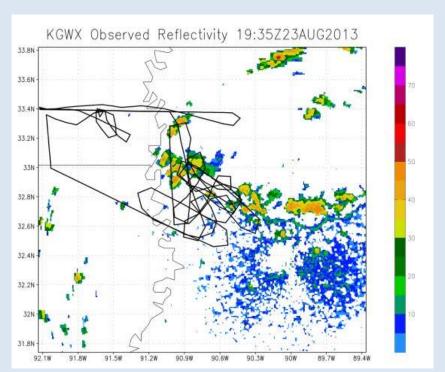
### Chemical Role of Deep Convection

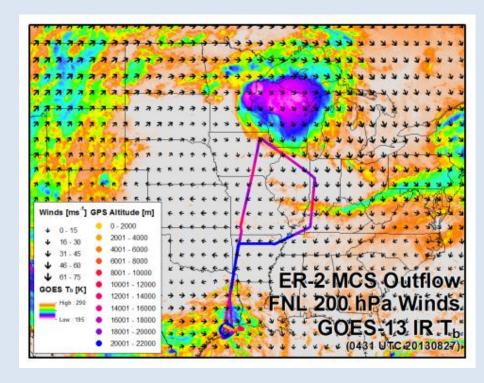
- Transports boundary layer air to UTLS
- Chemical transport as important as from warm conveyer belts of mid-latitude cyclones (Kiley and Fuelberg 2006)
- Generates lightning that produces nitrogen oxides (LNO<sub>x</sub>)
- If lofted, BL air abundant in CO, hydrocarbons, and peroxides reacts with NO<sub>x</sub> to produce upper tropospheric O<sub>3</sub> (Crutzen 1973; Chameides 1978; Pickering et al. 1996)
- LNO<sub>x</sub> is probable source of 70% of summertime upper tropospheric ozone in southern U.S. (SEAC<sup>4</sup>RS) (Cooper et al. 2007)

# General Objectives

- Use chemical transport model (WRF-Chem) to simulate at ~ 1 km resolution various SEAC<sup>4</sup>RS storms (single cells, multicells, continental, maritime)
- Focus on convective transport and chemical processes affecting O<sub>3</sub> and its precursors (e.g., NO<sub>x</sub>, OH, CO)
- Integrated research approach using simulations, airborne data, and satellite products

### **Example Storms**





SEAC<sup>4</sup>RS sampled many continental and maritime storms How do chemical transport signatures vary among the storms given that surface emissions will differ?

# Specific Questions

- Do simulated patterns and values of key chemical species and their fluxes compare to those observed in situ and by satellites?
- How do key species evolve during life cycle of convection?
- Are current LNO<sub>x</sub> parameterizations adequate? Can we improve them?
- How does the large vertical transport in convection change CO concentrations, affect O<sub>3</sub> concentrations, and the ability of the atmosphere to cleanse itself?

## Methodology—Model Selection

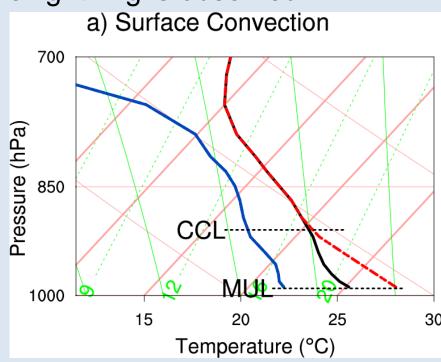
- Must faithfully depict chemical transport by deep convection
- WRF-Chem
  - Meteorological and chemical transport model
  - Use Regional Atmospheric Chemistry Mechanism (RACM)
- Run at convection permitting scales (~1 km)
  - Better matches scales of thunderstorms
  - Prevents diffusion of chemical concentrations (Heald et al. 2003; Lin et al. 2010)

# How to Estimate Lightning NO<sub>x</sub>

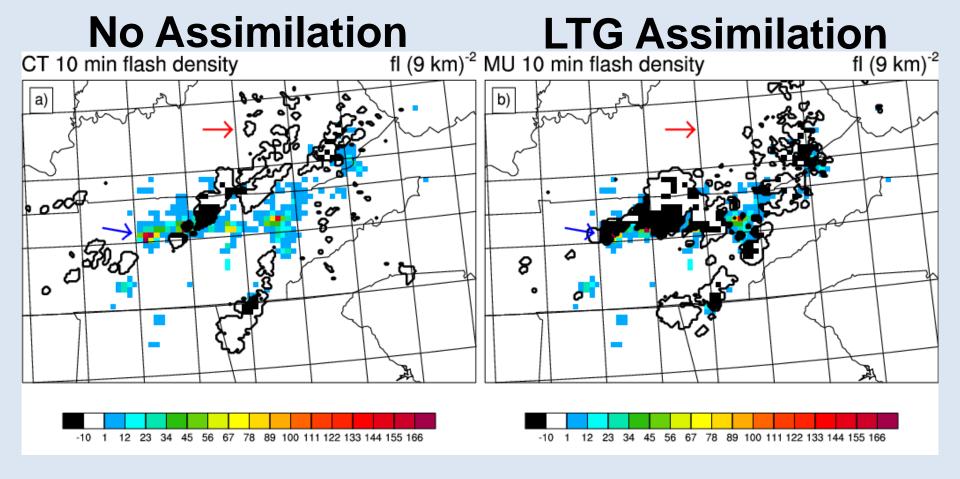
- LNO<sub>x</sub> parameterized based on:
  - Model fields of storm parameters (e.g., cloud top height, convective mass flux, max. vertical velocity, ice mass; Allen and Pickering 2002, Deierling et al. 2008, etc.)
  - Observed lightning fields (Kaynak et al. 2008, DeCaria et al. 2000, etc.)
- Mixed agreement with observations
- We want to develop even better parameterizations

## Lightning Data Assimilation

- Meteorological simulation improved by assimilating lightning data (Marchand and Fuelberg 2014)
  - Produces and locates storm where lightning is observed
- If observed lightning not simulated, we vary the T profile to initiate a storm <sup>®</sup>/<sub>2</sub>
- Nudging used in favor of variational/EnKF methods
- Difficult to initiate storm using Var/EnKF



#### Assimilation Results After 6 h



**Black** shading represents model agreement with observations: Black areas are good

### Develop Improved Data Assimilation

- Improve our method to better match observed storm intensity
  - SEAC<sup>4</sup>RS flight data (e.g., APR-2) to verify improvements
- Our method is effective at initiating deep convection, while 3D/4D-Var radar assimilation is effective at modulating convection
- Combine methods to improve meteorological simulation and, hence, chemical simulation

# **Experiment Configuration**

- Long duration simulations during SEAC<sup>4</sup>RS
- Control simulation without lightning assimilation. Consequently, LNO<sub>x</sub> could be placed where no deep convection is simulated
- 2) Simulation with our assimilation with LNO<sub>x</sub> from observed lightning
- 3) Simulation with our assimilation with LNO<sub>x</sub> parameterizations

# Summary

- SEAC<sup>4</sup>RS research will illustrate:
  - The vertical and horizontal distribution of O<sub>3</sub> and its precursors (NO<sub>x</sub>, OH, CO, etc.) in various storm types and their outflows
  - The importance of deep convective transport and LNO<sub>x</sub> generation for simulating O<sub>3</sub> concentrations
  - The importance of convective permitting scales for regional air quality modeling and potential deficiencies of climate models